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A Plot Twist in the Tale of Dental Cubic Zirconia—and a (Dis)course Correction

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Abstract

Different scientific fields occasionally have to deal with the problem of imprecision when definitions cross disciplinary boundaries and extend beyond the scope of technical oversight. This occurred when dentistry adopted ambiguous phase descriptions for zirconia materials from a ceramics community that was still grappling with methodological uncertainties. Here, we recount the origins of dental zirconia being mistakenly referred to as "cubic" as well as the reasons underlying the difficulties in accurately assessing crystallographic phase structures in such materials. We highlight compelling new evidence that corroborates earlier studies suggesting that zirconia within the compositional range of stabilization used in dentistry is fully tetragonal upon cooling from the sintering temperature.

Keywords: ceramics, biomaterial, polymorphism, ultrastructure, X-ray crystallography, physical properties

Introduction

It should come naturally to us to uphold the value of scientific expertise and precise terminology while remaining willing to revise our views when evidence demands it. A relevant example is zirconium dioxide (ZrO_2) used in prosthetic dentistry, typically stabilized with 3 to 6 mol% yttria (Y_2O_3). This yttria-stabilized zirconia (*x*YSZ) entered clinical practice with 3YSZ in the early 2000s and quickly became established. The remarkable transformation-toughening mechanism of 3YSZ, based on the tetragonal-to-monoclinic ($t \rightarrow m$) phase transformation, brought a sophisticated crystallographic concept into everyday dental terminology. With the introduction of more highly stabilized materials such as 4YSZ and 5YSZ around 2014, developed to improve translucency for monolithic restorations, these materials came to be widely described as "partly cubic zirconia." However, evidence shows that dental zirconia materials within the composition range $2.5 \leq x \leq 7.5$ are entirely tetragonal at room temperature when processed under conventional sintering and cooling conditions, as discussed below.

Lost in Translation

The first references in the dental literature to a cubic phase coexisting with the tetragonal phase can be traced back to the influential reviews by Denry and Kelly (2008) and Kelly and Denry (2008), both ranked among the most cited articles in the history of the journal *Dental Materials* (Rocha et al 2026). From there, the concept quickly spread throughout the dental community. The primary source (Chevalier et al 2004), however, leaned on spectroscopic measurements showing yttria enrichment of enlarged grains and depletion of neighboring small grains by prolonged sintering at 1,550 °C. They, in turn, supported their assumption of large grains being inevitably cubic by citing the transmission electron microscopy (TEM) images of Rühle et al (1984) and phase quantifications by X-ray diffraction performed by Ruiz and Readey (1996) and later by Matsui et al (2003). Although Ruiz and Readey (1996) showed a phase identified as cubic increasing in content following the increase in grain size with temperature, their fully submicrometric starting material was determined to already comprise a *c*-phase in 25 mass%; their fully coarsened material retained 62 mass% of *t*-phase, indicating that grain size alone could not be indicative of phase structure. A similar trend of increasing *c*-phase with grain size in 3YSZ was observed by Matsui et al (2003), which detected Y^{3+} migration toward grain boundaries and triple junctions, thus inferring a $t \rightarrow c$ diffusive transformation. In Chevalier et al (2004), attention was brought to the fact that such a dual microstructure containing both a Y-rich cubic and a Y-lean tetragonal polymorphs could be predicted from the phase diagram of Scott (1975), shown truncated at greater than 1,250 °C at the $t+c$ metastable field.

Difficulties in distinguishing *t* and *c* phases from a low-tetragonality high-yttria tetragonal variant (t') appearing via cooling from above or within the metastable *c*-field were known by then (e.g., Scott 1975; Chaim et al 1985; Lanteri et al 1986; Zhou and Lei 1991; Sanchez-Bajo et al 1992; Sheu et al 1992). Especially using conventional low-resolution X-ray diffraction (XRD) equipment that employs a mixture of $CuK\alpha_1$ and $CuK\alpha_2$ radiation, the t' and *c* phases give a strong overlap at both intermediate and high angular regions where

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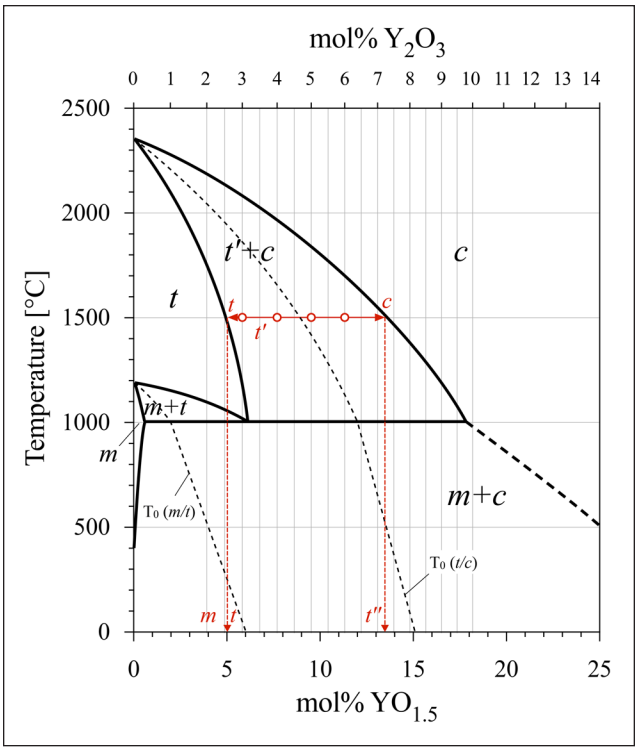

Figure 1. ZrO_2-Y_2O_3 phase diagram with typical dental zirconia compositions (3-6YSZ, circles) sintered at 1,500 °C with hypothetical decompositions toward the *t*- and *c*-phase boundaries and transformations upon cooling (modified from Fabrichnaya et al 2005). As a practical example, 4YSZ could decompose at 1,500 °C in both a Y-lean *t* phase and a Y-rich *c* phase (horizontal shift along the *x*-axis). Upon cooling to room temperature, some now *c* phase would further transform into the very-low-tetragonality polymorph *t*″.

the peak intensity is particularly low. Improved Rietveld refinement strategies (Sanchez-Bajo et al 1997) and the use of high-intensity diffractometers monochromated to remove the $K\alpha_2$ component were thus recommended to resolve phase assignment and improve phase fraction quantification (Gibson and Irvine 2001). The use of XRD poses a problem because it is less sensitive to the perturbations induced by the component of the tetragonality distortion stemming from the anion cage. This can lead to the cubic phase being identified by XRD (Krogstad, Lepple, et al 2011; Krogstad et al 2013; Lipkin et al 2013; Krogstad et al 2015), as opposed to, for example, electron diffraction; TEM studies have confirmed this for compositions <7.5mol% Y_2O_3, where solely the Y-rich tetragonal variant appears (Sheu et al 1992; Krogstad, Lepple, et al 2011), including dental 3YSZs where no *c*-phase is seen (Grigore et al 2013).

Regardless of analytical intricacies, the composite structure of Y-stabilized zirconia is complex since it can segregate in phases that inhabit several phase fields and go through phase boundary transitions upon sintering and cooling; the decomposition into distinct variants and other phases has been shown to depend, among other things, on the chemical homogeneity of the starting material, thermal history, and cooling rate (Krogstad, Lepple, et al 2011). More recent analyses (Krogstad et al 2013; Lipkin et al 2013; Krogstad et al 2015) reveal increasing microstructural complexity and thermodynamic phase evolution, describing up to 3 tetragonal variants: *t*, *t*′, and *t*″. The variant termed *t* is the high-tetragonality (c/a ~ 1.015) Y-lean equilibrium phase (the transformable to *m* symmetry). The one described as *t*″ has a very low tetragonality (c/a ~1.005) and is the actual confounding with the cubic phase that ensues from a high-temperature *c*-phase cooling down through the $T_0(t/c)$ line in Figure 1. The phase first termed *t*′, reminiscent at room temperature, has been recently posited to be rather an artifact from the coherency strain between the decomposition by-product phases (Krogstad, Krämer, et al 2011; Krogstad et al 2015). There is no question that the inclusion of more phases during XRD refinement will improve the fitting, but it seems equally sound by today's interpretations that any identifiable *c*-phase in compositions below ~7.5 mol% Y_2O_3 corresponds in fact to a low-tetragonality structural variant.

This being largely unbeknownst in the dental community, the notion of dental zirconia containing a cubic phase got traction with other seminal papers suggesting that the higher translucency of 4YSZ and 5YSZ materials is achieved through the introduction of increased amounts of the nonbirefringent cubic phase (Zhang 2014) that grows into larger grain sizes reducing grain-boundary scattering (Zhang and Lawn 2018). However cautiously, the referencing of zirconia products being based on "cubic zirconia" did not hurt manufacturers pushing for market share of new "translucent" monoliths and multilayer structure-graded materials for broader clinical indication. In the meantime, studies caught up with methodological nuances and began adopting technical upgrades along with suitable evaluations based on a 2-tetragonal model that excludes the cubic premise (Belli et al 2021; Harada et al 2020; Nakamura et al 2024). In this issue of *JDR*, Nakamura et al (2026) present a noteworthy effort to overcome uncertainties inherent to laboratory X-ray diffractometers and confirm evidence from outside the field (Lipkin et al 2013) to resolve this debate for the dental community: they seized on the inherently high intensity of synchrotron radiation to accurately assign phase structures in typical 3-8YSZ feedstocks used in dentistry while giving further insights into atomistic ordering and low-temperature degradation effects.

A Way Forward

This brief historical account is not intended to trivialize the many advances achieved by dental research and industry over the past 25 y nor to overstate the importance of material categorization. Rather, we hope it will encourage the community to reassess its commitment to rigor when translating concepts from other disciplines and communicating them to students and practicing dentists. The latter task is not trivial, given the continuous involvement of intermediaries—such as industry representatives, salespeople, and dental technicians—who understandably seek to break down technical terminology into more accessible language. If referring to the spectrum of tetragonality when distinguishing among zirconia materials proves too abstruse, the straightforward designation xYSZ

(e.g., 3YSZ, 4YSZ, 5YSZ, 6YSZ, and combinations thereof in graded products—all fully tetragonal) provides a clear and unambiguous alternative.

Regardless of how the field ultimately chooses to address this issue, it remains mainly academic and bears no direct effect on clinical outcome. More concerning is the gamble being taken by prioritizing optical over mechanical performance through the widespread and largely unrestricted use of 4-6YSZs; the fallout could prove far more costly, say, to the cube.

Author Contributions

R. Belli, contributed to conception and design, data acquisition and interpretation, drafted and critically revised the manuscript; U. Lohbauer, contributed to conception and design, data interpretation, drafted and critically revised the manuscript. All authors gave their final approval and agree to be accountable for all aspects of the work.

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